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Author(s): Grove, John W.

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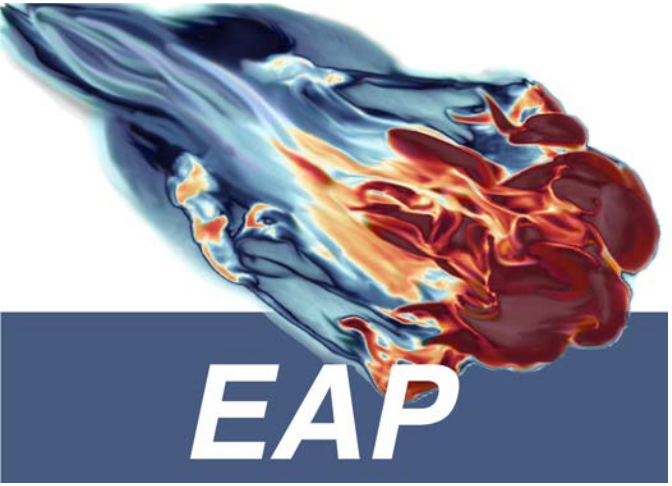
Eulerian Applications Project - xRage



The xRage Equation of State: Input Options

John W. Grove
CCS-2

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NNSA National Nuclear Security Administration

Table Creation Options

Name	Type	Name	Type
teos_file	character string	pscale_neg	real
sesfiles	character string array	numprsdec_pos	integer
mat_sesfiles	character string array	numprsdec_neg	integer
numm	integer	numtev_tension	integer
matid	integer array	tevhi_tension	real
matdef	rank two real array	force_cold	logical
matident	character string array	teos_noextrapolate	logical
eostype	integer array	use_thermoderivs	logical
use_shared_memory	logical	use_eos_direct	logical
prslo	real	mxdome_itr	integer
prshi	real	do_sesame_edit	logical
numprsdec	integer	debug_eos_inv_t	logical
tevlo	real	test_tabbld	logical
tevhi	real	test_pt_inversion	logical
numtevdec	integer	list_crossed	logical
support_tension	logical	print_shared_teos_data	logical
pscale	real	debug_eos_model	logical
pscale_pos	real	high_T_emin	real

Table Creation Debugging Options

Name	Type	Name	Type
debug_eos_inv	logical	print_shared_teos_data	logical
test_tabbld	logical	debug_eos_model	logical
test_pt_inversion	logical	high_T_emin	real
list_crossed	logical		

EOS Table Creation Options The Whole Shebang Commonly Used General Options

- **teos_file** – the name to be used for the EOS table file
- **sesfiles** – an array of file names with locations to look for sesame files
- **mat_sesfile** - an array of filenames that will be used for specific materials
- **numm** – integer, the number of materials to be inserted in the EOS file
- **matid** – integer array of material ids these will be used in the simulation input file to identify materials
- **matdef** – dimension two real array an array for EOS parameters
- **matident** – character string array, symbolic names for materials
- **eostype** – integer array, specifies the equation of state model to be used for a material
- **use_shared_memory** – logical scalar (default=false) when true the storage for the EOS table will use MPI shared memory. This reduces the amount of storage needed for the table by a factor of the size of a shared memory node.

EOS Table Creation Options The Whole Shebang Commonly Used Table Lattice Options

- **prslo**, **prshi**
  - The pressure range for the created table. EOS data is computed for pressures in the range $prslo \leq P \leq prshi$
  - defaults prslo = 10^4 microbars, prshi = 1.5×10^{22} microbars
- **numprsdec** (20)
  - controls the number of tabulated pressures
  - numprsdec decades starting at prslo > 0
    - recommendation – use a value of 80 or bigger
  - If prslo>0 pressure points are created at

$$p(n) = \text{prslo}\times10^{\frac{n-1}{\text{numprsdec}}}\ 1 \leq n \leq 1 + \text{numprsdec}\times log_{10}\left(\frac{\text{prshi}}{\text{prslo}}\right)$$

- **tevlo tevhi**
  - The temperature range for the created table. EOS data is computed for temperatures in the range $tevlo \leq T \leq tevhi$
  - defaults tevlo = 0.01 eV/k ≈ 116.04522 K, tevhi = 10^6 eV/k ≈ 1.16×10^{10} K
- **numtevdec** (20)
  - controls the number of tabulated temperatures
  - numtev decades starting at tevlo
    - recommendation – use a value of 80 or bigger

Equation of State Creation Options
The Whole Shebang – Tension Support Options

- **support_tension**, (default=false) when true allows a non-positive value for prslo
  - The value of this variable is recorded in teos_file and read when running an application. A user can disable this option by setting support_tension=.false. in their application input file
- The pressure grid for support_tension is controlled by three input options
  - **pscale** (10^4 microbars), **pscale_pos**, and **pscale_neg** - the default value for pscale_pos and pscale_neg is pscale
- **numprsdec_pos**, **numpresdec_neg** control the number of pressure points to be inserted in the grid. Their default value is **numprsdec.**
  - The pressure values inserted will be
    - $p(n) = -\text{pscale\_neg} \cdot 10^{\frac{nump_{neg}+1-n}{\text{numprsdec\_neg}}}, -\text{pscale\_neg} \cdot 10^{\frac{nump_{neg}+1-n}{\text{numprsdec\_neg}}}, 1 \leq n \leq nump_{neg}$
    - $p\left(nump_{neg}+1\right) = 0$
    - $p(n) = \text{pscale\_pos} \cdot 10^{\frac{n-(nump_{neg}+1)}{\text{numprsdec\_pos}}}, \text{pscale\_pos} \cdot 10^{\frac{n-(nump_{neg}+1)}{\text{numprsdec\_pos}}}$
  - An additional point at the standard pressure of one bar will also be inserted in the table

Equation of State Creation Options
The Whole Shebang – Temperature Grid Control

- The temperature grid is also a logarithmic grid similar to the pressure grid with some important differences
- If support_tension is false the temperature grid is given by
  - tevlo>0

$$t(n) = \text{tevlo} \times 10^{\frac{n-1}{\text{numtevdec}}}, 1 \le n \le num_{tev} = 1 + \log_{10}\left(\frac{\text{tevhi}}{\text{tevlo}}\right)$$

  - tevlo=0

$$t(n) = \text{tevhi}\,\frac{10^{\frac{n-1}{\text{numtevdec}}-1}}{\text{tevhi}+1}, 1 \le n \le num_{tev} = 1+\text{numtevdec} \times \log_{10}(1+\text{tev}hi)$$

- If support_tension is true the above points will be inserted into the grid and an additional linear section of temperature are inserted controlled by the input specifications **numtev_tension** and **tevhi_tension** at a constant interval of $\Delta t = \frac{\text{tevhi\_tension}-1}{\text{numtev\_tension}_{-1}}$
- Two additional points may be inserted
  - A room temperature point is always inserted at 0.025 eV/k = 290.11305 K
  - If the input directive **force_cold** (false) is true a temperature point at the value 10^{-6} eV/k = 0.011604522 K will be inserted into the temperature grid.

Equation of State Creation Options
The Whole Shebang – Other Table Creation Options

- **teos_noextrapolate** (false) – this is a directive used internally by the table evaluation code to disable any extrapolations outside the table domain $prslo \leq P \leq prshi, tevlo \leq T \leq tevhi$ this variable is recorded in the teos_file and can be reset in the application input file
- **use_thermoderivs** (false) – this option tells the tabular EOS evaluator to use a special routine to compute derivatives.
- **use_eos_direct** (false) - this directive sets up the ability to perform pure material evaluations via their analytic equation of state formulas or in the case of Sesame to use EOSPAC to evaluate the equation of state. It also affects the construction of the table. When true the values for support_tension and teos_noextrapolate are also set to true. The value of this directive is also stored in teos_file and can be reset in the application input deck.
  - When used this option will compute default values for prslo, prshi, tevlo, and tevhi based on the domain limits of the individual EOS models. The values can be overridden by input file values.

Equation of State Creation Options
The Whole Shebang – Sesame Related Options

- **eostype(mat)** – selects when pressure-temperature inversion tool to use when computing an EOS table for Sesame
  - **eostype(mat) = 99** (default) – use EOSPAC to invert the Sesame table
  - **eostype(mat) = 0** – use the xRage provided routines to invert the Sesame table
- **sesfiles** – an array of file names with locations to look for sesame files
- **mat_sesfile** - an array of filenames that will be used for specific materials
- **eostype(mat) = 0** only options
  - **mxdome_itr** (10000) – sets a maximum for the number of iterations to be used when computing the vapor dome for a sesame material
  - **do_sesame_edit** – turns on diagnostic printing when computing the vapor dome for a sesame material

Equation of State Creation Options
The Whole Shebang – Debugging Options

- **debug_eos_inv_t** (false) – turns on diagnostic output for the inversion of the equation of state models into pressure-temperature form. May produce copious output.
- **test_tabbld** (false) – After the EOS table is created run the routine teos_load_select to create an EOS evaluation object and test the evaluation by calling the EOS at the table points. The EOS usage options apply. Produces a lot of output much of which is in separate files.
- **test_pt_inversion** (false) – prints diagnostics about the pressure-temperature inversion routines.
- **list_crossed** (false) – prints a list of any crossed pressure-density isotherms found during table inversion
- **print_shared_teos_data** (false)) – prints a summary of the shared memory data structures.
- **debug_eos_model** (false) – print debugging information for the inversion into pressure-temperature form.
- **high_T_emin** (0,–∞ if teos_noextrapolate is true) – EOS table checking will fail if the specific internal energy at the maximum temperature on an isobar is less that this value.

EOS Usage Options:

Name	Type	Name	Type
keos	integer	sie_min	real
eosfile	character string	enforce_sie_min	logical
eostype	integer array	rho_min	real
nummat	integer	enforce_rho_min	real
daltonmix	logical	pmin_mat	real array
matdef	rank 2 real array	pfail_mat	real array
matident	character string array		
use_eos_intrinsic_inversion	logical	void_mat	integer
VERY_COLD	real	true_void	logical
MAXIMUM_DENSITY	real	void_prs	real
MINIMUM_PRESSURE	real	void_rho	real
MAXIMUM_PRESSURE	real	void_tev	real
NONZERO_SOUND_SPEED_DENSITY_FLOOR	real	void_sie	real
ROEPS	real	VOID_CELL_TOL	real
snd_max	real		

Equation of State Usage Options

- After creating an equation of state file as outlined in the previous set of slides there are a number of options that can be exercised when using that EOS file in an application. The following outlines these options.
- **hydro_version** (-1 no hydro version) - This is not really an equation of state option, but if a value is used for a non-equilibrium hydrodynamic option the effect of EOS calls can be changed.
- **eosfile** (empty) – when provided this input option gives the name of the file where the tabulated pressure-temperature equation of state is located. It will generally be the same name used when creating the EOS file as given by to teos_file option.
- **eostype** (99 use EOSPAC for PT inversion) – this option defines the equation of state models to be used. When using a PT tabular equation this array is printed in eosfile and this value is used to initialize the array.

Equation of State Usage Options

- **nummat** – the number of materials to be used in an application
- **daltonmix** (false) – when true the EOS for a mixture will be based on molecular (Dalton) rather than Amagat mixtures.
- **matdef** – provides EOS and other parameters
  - **matdef(1,mat)** provides the material id to be used to find the EOS data. This value should be the same as the corresponding matid used in the TEOS generation input
  - **matdef(5,mat)** sets the minimum allowed pressure for a material
  - **matdef(25,mat)** scales the densities in the PT table for material mat
  - **matdef(26,mat)** when keos=3 provides a specific internal energy offset for the table data
    - When using keos different from 3 this is the minimum allowed temperature for the analytic model being used
  - **matdef(90,mat)** when using Dalton mixtures cells will material mat will be treated using Amagat mixtures
  - When using the direct eos options, EOS parameters are written in eosfile and used to set the values for the individual models
- **matident** (as read from eosfile) - provides a symbolic name for materials

Equation of State Domain options

- **VERY_COLD** (10^{-6} eV/k $\approx$ 0.011604522 °K) – This option sets a floor on temperature.
- **MAXIMUM_DENSITY** ($+\infty$) – sets a ceiling on allowed densities
- **MINIMUM_PRESSURE** ($-\infty$) – sets a floor on allowed pressures
- **MAXIMUM_PRESSURE** ($+\infty$) – sets a ceiling on allowed pressures
- **NONZERO_SOUND_SPEED_DENSITY_FLOOR** – sets a floor for sound speed. Any computed sound speeds below this value are set to zero
- **ROEPS** (10^{-15}) – this is a floor for the mass fraction of a component in a mixture. Components with mass fraction less than this value are removed from the mixture.
- **sie_min** (0), **enforce_sie_min** (false) – When enforce_sie_min is true specific energies for material mat are floored at sie_min(mat).
- **rho_min** (0), **enforce_rho_min** (false) – When enforce_rho_min is true densities for material mat are floored at rho_min(mat).
- **pmin_mat, pfail_mat** ($-\infty$) – These options are the same and set a minimum allowed pressure of each material
- **snd_max** (huge(ONE)) – sets the maximum allowed sound speed

Equation of State options: Void

- **void_mat** (0) - use this material as the void material
- **ture_void** (false) – When true the void material will have zero mass
- A property of the void material is that the thermodynamics of void are constant
- **void_prs** (0) – specifies the pressure of the void material
- **void_rho** (0) – the density of the void material
- **void_tev** (0) – the temperature of the void material
- **void_sie** (0) – the specific internal energy of the void material
- **VOID_CELL_TOL** (1) – when the volume fraction for the void material is greater than or equal to VOID_CELL_TOL treat the cell as only containing void

EOS Table Evaluation Options

Name	Type	Name	Type
MAX_ITER_TEOS	integer	use_eos_direct	logical
MAXBINARY	integer	support_tension	logical
TEOS_CONVERGENCE_TOL	real	use_thermoderivs	logical
DENSITY_TOL	real	teos_noextrapolate	logical
PRESSURE_TOL	real	ramp_num	integer
VOL_TOL	real	ramp_mat	integer array
SIE_TOL	real	ramp_alpha	real array
TEMPERATURE_TOL	real	ramp_pe	real array
MIN_P	real	ramp_pc	real array
MIN_SIE	real	ramp_pe_de	real array
use_teos_iter_5	logical	ramp_pc_de	real array
teos_secant	logical	ramp_reverse	logical array
secant_fix	logical	ramp_model	integer
do_not_push_pres	logical	ramp_coef	real array
use_eos_direct_pte	logical	ramp_power	real array
try_eos_direct_ramp	logical	ramp_pe_eng	real array
eospac_bilinear	logical	ramp_pc_eng	real array
eospac_invert_at_setup	logical	ramp_T0	real array
eospac_eos_insert_data	logical	ramp_P0	real array
use_simplified_teos	logical	ramp_rho0	real array
use_shared_memory	logical		

Tabular Equation of State Usage Options

- **use_simplified_teos** (false) – use an alternative implementation of the tabular EOS solver. Algorithmically the same as the default method, but used an array based implementation.
- **use_shared_memory** (false) - When true the storage of the pressure-temperature tables use MPI shared memory.
- **use_eos_direct** (as read from eosfile) – this option can be used in the application input file to turn off the use of the direct eos evaluation option. It cannot be turned on in this way. The user must request this option in the teos file generation input.
- **support_tension** (as read from eosfile) – allow negative pressures
- **use_thermoderivs** (true if use_eos_direct is true false otherwise) – use a special routine to compute thermodynamic derivatives
- **teos_noextrapolate** (as read from eosfile) – avoid extrapolations in pressure-temperature space
- **use_eos_intrinsic_inversion** (false) – this option is primarily for initialization. When true a density-temperature evaluation will use the intrinsic capabilities provided by the EOS solver. When false a bisection root finder will be used to invert the energy-density EOS into a temperature-density evaluation. When running the **xmeos_invert_test**, this option is called **intrinsic_rhoe**, which is true by default.

Equation of State – PT Solver Options

- **MAXITER_TEOS** (100) – Number of iterations to use for the PT root finder
- **MAXBINARY** (MAXITER_TEOS/5) – After MAXITER_TEOS iterations attempting to find the PT solution perform MAXBINARY iteractions of a bisection method
- **TEOS_CONVERGENCE_TOL** (10^{-12}) – A generic unitless value for measuring relative convergence of the PT root finder
- **DENSITY_TOL, PRESSURE_TOL** (TEOS_CONVERGENCE_TOL) – The EOS is said to converge if the relative difference between the current and previous iteration values of density and pressure are below their respective tolerance
- **VOL_TOL, SIE_TOL** (TEOS_CONVERGENCE_TOL) – If support_tension or teos_noextrapolate are true convergence occurs when the relative difference between the current and desired specifc volume and specific internal energy are below their respective tolerance
- **TEMPERATURE_TOL** (TEOS_CONVERGENCE_TOL) – Declare the computed PT solution converged if the temperature and pressure differences between the bounding table values are below their respective tolerances
- **MIN_P** (1 μbar) - this is a floor for relative absolute value of pressure differences
- **MIN_SIE** (1 $erg/gram$) – a floor for relative absolute value of specific internal energy differences.

Equation of State Usage Options – Experimental Options

- **use_teos_iter_5** (false) – uses an alternate mixture solver that is designed for improved speed and robustness
- **teos_secant** (false) – an obsolete option that uses a secant based solver and bilinear interpolation of the EOS tables
- **secant_fix** (false) – if the standard EOS solver did not converge attempt to compute the EOS using the secant method outlined above
- **do_not_push_pres** (false) – don't attempt to push out of domain pressures back into domain
- **use_eos_direct_pte** (false) – try to compute Amagat mixtures using the direct component EOS models. By default these mixtures are computed using the PT EOS tables.
- **try_eos_direct_ramp** (false) – an experimental option to compute ramp equations of state using the direct eos evaluations.

Equation of State Usage Options - EOSPAC options

- This list of options apply when using the test_tabbld option
- **eospac_bilinear** (false) – use the bilinear interpolation option in EOSPAC instead of the default rational interpolation option
- **eospac_invert_at_setup** (false) – use the EOS evaluation acceleration option invert at setup when evaluating a Sesame table with EOSPAC
- **eospac_eos_insert_data** (0)– Sets the EOSPAC option EOS_INSERT_DATA. When positive EOSPAC will insert eospac_eos_insert_data additional points between each of the data points used by for evaluating a table.

Equation of State: Porous Ramp Model

- The EOS for a material can be modified using a porous ramp model
- Inside the ramp the evaluated specific volume and specific internal energy are given by

$$V_{ramp}(P,T) = \alpha(P) V_{table}(P,T)$$

$$e_{ramp}(P,T) = e_{table}(P,T) - \left\{ \left(\frac{\alpha(P) - 1}{\alpha_{pe} - 1} \right) \Delta_{pe} e + \left(\frac{\alpha_{pe} - \alpha(P)}{\alpha_{pe} - 1} \right) \Delta_{pc} e \right\}$$

- The formula for $\alpha(P)$ depends on whether the ramp is reversible or not
- Reversible ramp

$$\alpha(P) = \begin{cases} \alpha_{pe} & , P \le P_e \\ \alpha_{pe} + \dfrac{P - P_e}{P_c - P_e}\left(1 - \alpha_{pe}\right) & , P_e \le P \le P_c \\ 1 & , P_c \le P \end{cases}$$

- Irreversible ramp – replace the value of P in the above equation by $\max(P, P_{max})$, where P_{max} is the maximum pressure encountered in the fluid particle
- Physically $\alpha(P)$ is the reciprocal of the solid component volume fraction

Porous Ramp Input

- **ramp_num** (0) – the number of materials for which ramp modifications are to be installed
- **ramp_mat** (0) – an array of ramp_num material indices for which are to use a ramp modification
- **ramp_alpha** (0) – an array of ramp_num values for the quantity α_{pe}
- **ramp_pe** (0) – ramp_num array for the values P_e
- **ramp_pc** (0) – ramp_num array for the values P_c
- **ramp_pe_de** (0) – ramp_num array for the values $\Delta_{pe}e$
- **ramp_pc_de** (0) – ramp_num array for the values $\Delta_{pc}e$
- **ramp_reverse** (false) – ramp_num array indicating whether the ramp for that material is reversible
- Note: The above arrays are read from the input file as ramp_num arrays, but are converted internally into nummat arrays.

Porous Ramp Model: Ramp Model 2

- An alternate version of the porous ramp model is also available to exercise this option the input file directive
- **ramp_model** (1) - specify the porous ramp model, should be set to 2

The following input controls are common with ramp model 1

- **ramp_num , ramp_pe, ramp_pc, ramp_mat, ramp_alpha**
- Controls specific to ramp model 2 are:
- **ramp_coef** (0) – ramp_num array of coefficients, ramp_coef(mat)≤ 1
- **ramp_power** (2) – ramp_num array of exponents for the ramp formulas
- **ramp_pe_eng** (0) – ramp_num array of non-negative ramp energy offsets
- **ramp_pc_eng** (0) – ramp_num array of non-negative ramp energy offsets
- **ramp_T0** (0), **ramp_P0** (0), **ramp_rho0** (0) – Thermodynamic variables to set the value of ramp_alpha automatically. If all three are positive, the value for ramp_alpha is given by

$$\alpha_{pe} = \frac{\rho_s(P_0, T_0)}{\rho_0}$$

  evaluated at each ramp material.
- As with ramp_model = 1, these values are read are read from input as ramp_num arrays and converted internally into nummat arrays.

Ramp Model 2: Formulas

- Notation: For simplicity we do not denote material dependence
  - ramp_alpha = α_{pe} , ramp_coef = C_r, ramp_power = p, ramp_pe_eng = e_{pe}, ramp_pc_eng = e_{pc}
- $e_{ramp}(P,T) = e_{table}(P,T) + \Delta e_{ramp}(P)$

$$\Delta e_{ramp}(P) = \begin{cases} e_{pe} & \max(P, P_{max}) \le P_e \\ e_{pe} + \left(\frac{e_{pc}-e_{pe}}{P_c-P_e}\right)(\max(P, P_{max}) - P_e) & P_e \le \max(P, P_{max}) \le P_c \\ e_{pc} & P_c \le \max(P, P_{max}) \end{cases}$$

- In contrast to ramp model 1 the energy offset in linear in pressure rather than alpha
- If C_r=0 $\alpha(P)$ is the same as for an irreversible ramp for model 1
- The ramp coeficient and ramp power satisfy $C_r \le 1 < p$

$$\alpha(P) = \begin{cases} \alpha_{pe} & \max(P, P_{max}) \le P_e \\ \alpha_{pe} + C_1 s + C_2 s^p & P_e \le \max(P, P_{max}) \le P_c,\ s = \frac{max(P,P_{max})-P_e}{P_c-P_e} \\ 1 & P_c \le \max(P, P_{max}) \end{cases}$$

$$C_1 = (1-\alpha_{pe})w,\ C_2 = (1-\alpha_{pe})(1-w),\ w = \begin{cases} \frac{1-C_r}{p-1} & C_r < 0 \\ 1-C_r & C_r > 0 \end{cases}$$

Other Options

- Non Equilibrium Options

Name	Type	Name	Type
eos_select	integer	tev_average	integer
pte_mat	integer array	single_pressure_multiple_temperature_eos	logical

- Atomic Mass/Atomic Number

Name	Type	Name	Type
abar	real	zbar	real

- Diagnostics/Debugging

Name	Type	Name	Type
debug_eos	logical	debug_teos_p_vol	logical
check_eos	logical	write_eos_domain	logical
debug_eos_direct	logical	write_eos_convergence_results	logical
check_snd_max	logical		

Non-equilbirum Equation of State Usage Options

- **eos_select** (0) – specifies the use of one of a variety of EOS mixtures treatments
  - **eos_select=0** – use pressure-temperature equilibrium (Amagat) mixtures
  - **eos_select= 60** – use a thermal isolation non-equilibrium model (equilibrated pressure advection of component specific entropy)
  - **eos_select=61** – use a uniform compression mixture model (equilibrated pressure advection of material mass fraction)
  - **eos_select=14** – use a multiple pressure mutiple temperature mixture model
  - **eos_select=80** – used an EOS model modified to treat plasmas
- **pte_mat(mat)** (false) – when using a non-equilibrium EOS option mixtures containing this material are to be treated as Amagat mixtures
- **tev_average** (3) – specifies how an average temperature is to be computed for a non-equilibrium mixtures
  - **tev_average=3** – specific heat weighted average
  - **tev_average=2** – mass weighted average
  - **tev_average=1** – volume fraction average

Equation of State Options: atomic data

- **abar** – (0 or read from sesame) – Material atomic mass
- **zbar** – (0 or read from sesame) – Material atomic number
- Attempts to set default values for analytic models are made based on an ideal gas approximation abar = $\frac{R}{\Gamma C_V}$ where R is the universal gas constant. There is not good guess for zbar.

Equation of State Usage Options – Debugging Options

- **debug_eos** (false) – turns on diagnostic output for the table setup process and EOS evaluations when test_tabbld is true. Will produce copious output, use with care.
- **check_eos** (false) – turns on diagnostic tests for valid EOS evaluations
- **debug_eos_direct** – (false) – prints diagnostics for the direct eos option initialization
- **check_eos_domain** (false) – turns on checking for EOS domain
- **check_snd_max** (false) – turns on checking that the evaluated sound speed doesn't exceed snd_max
- **debug_teos_p_vol** (false) – obsolete unused option
- **write_eos_domain** (false) – when true the equation of state domain for each model will be printed
- **write_eos_convergence_results** (false) – when true write a report for each EOS call on the convergence of the pressure-temperature equilibrium computation

Tabular EOS Test

- **teos_test** (false) – reads an eos table and tests evaluations
  - EOS inputs used
    - eosfile, nummat, matdef
  - Internal inputs
    - **tevlo, tevhi, prslo, prshi** (0) – limits for the evaluation grid
    - **fm** (0) – component mass fractions
    - **numdec** (0) – number of pressure decades to evaluation
    - **doall** (false) – sets the defaults for the evaluation grid to the table limits read from eosfile
    - **dofine** (false) – when true the evaluation metric for pressure and temperature are used for diagnostics
    - **donew** (false) – unused
    - **doedit** (false) – print evaluation error metrics
    - **doslow** (false) – add evaluations at zero pressure and temperature

EOS Tests

- **bmod_test** (false) – test the evaluation of the equation of state and the value for the bulk moduli
  - **prs** (10^6 μbar) – pressure where the evaluation will be performed
  - **tev** (0.025 eV/k) – temperature for the evaluation
  - Other inputs are used to set up the equation of state model
- **xmeos_MT_test** (false) – Test the multiple temperature single pressue equation of state model on a perfect gas/stiff gamma law mixture
  - **numstate** (1) – number of evaluations to perform
  - **e, V, mass_fraction** (0) – specific internal energy, specific volume, and mass_fractions for the components

EOS Tests

- **xmeos_RS_test** (false) – Construct a random sample of states using a Latin hyper cube and evaluate the PT mixtures
  - **numstates** (0) – number of states to evaluate
  - **log_lhc** (false) – build the latin hypercube in log space
  - **eosoutfile** ('RANDOM_EOS') – file name for the output
  - **rholo, rhohi** ($\infty, -\infty$) - density range to evaluate
  - **sielo, siehi** ($\infty, -\infty$) - specific internal energy range
  - **fmlo, fmhi** (0, 1) – mass fraction range
- **xmeos_eval_test** (false) – test the EOS evaluation for both pressure-temperature equilibrium and molecular mix
  - **rho** (0) – density
  - **sie** () – specific internal energy
  - **fm** (0)– mass fraction
- **test_gruneisen2** (false) –
  - **debug_gruneisen2** (false) -

EOS Tests

- **xmeos_invert_test** (false) – test the EOS evaluation for input based on pressure and temperature, density and energy, pressure and density, and density temperature
  - **rho** (0) – density
  - **sie** (0) – specific internal energy
  - **prs** (0) – pressure
  - **tev** (0) – temperature
  - **pmx** (0) – maximum pressure
  - **fm** (0)– mass fraction
  - **mat** (1) – material index for a pure state evaluation
- **test_gruneisen2** (false) – Evaluate the Grüneisen EOS for all data in Steinberg's report
  - **debug_gruneisen2** (false) – turn on internal debugging for the EOS evaluations

Obsolete Options

- Table Creation

Name	Type	Name	Type
auto_teos	logical	plot_emin	real
dorawplots	logical	plot_emax	real
plot	logical	plot_tmin	real
dolog	logical	plot_tmax	real
plot_rmin	real	plot_vmin	real
plot_rmax	real	plot_vmax	real
plot_pmin	real		
plot_pmax	real		

- Other Options

Name	Type	Name	Type
use_special_p_scaling	logical	use_old_ss	logical
MULTI_T_TOL	real	scale_p_mat	real array
FAST_MT_EOS	logical		

Obsolete or Seldom Used Equation of State Options

- **auto_teos** (false) – attempt to set up the pressure-temperature grid automatically
- **dorawplots** (false) – obsolete
- **plot** (false) – obsolete
- **dolog** (false) – obsolete
- plot_ints () – obsolete
- **plot_rmin, plot_rmax, plot_pmin, plot_pmax, plot_emin, plot_emax, plot_tmin, plot_tmax, plot_vmin, plot_vmax** – obsolete
- **use_special_p_scaling** (false) – obsolete
- **MULTI_T_TOL** (10^{-2}) – convergence tolerance for the single-pressure multiple temperature mix model. Convergence is based on the desired specific internal energy and the material pressure
- **FAST_MT_EOS** (true) – when true only perform one MT iteration
- **single_pressure_multiple_temperature_eos** (false) – when true the multiple temperature and multiple pressure EOS will impose pressure equilibrium
- **use_old_ss** (false) – provided for backwards compatibility. Use an old incorrect formula for the mixture sound speed
- **scale_p_mat** (1) – allows to user to provide a desired pressure scaling for a material.